Discovery of an Inhibitor of the Rpn11 Proteasome Subunit

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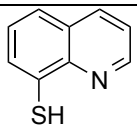
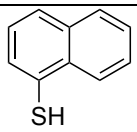
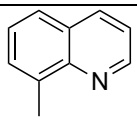
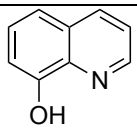
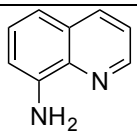
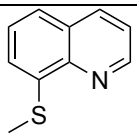
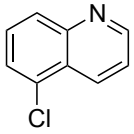
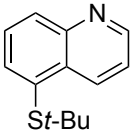
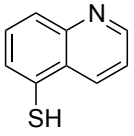
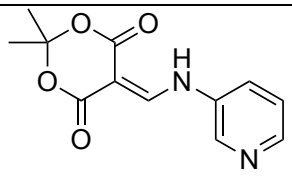
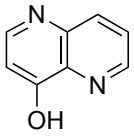
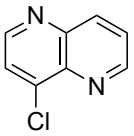
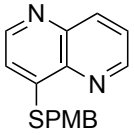
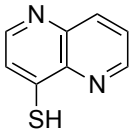
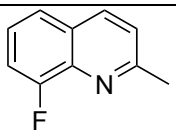
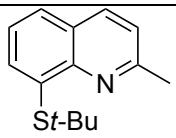
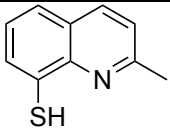
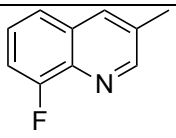
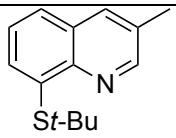
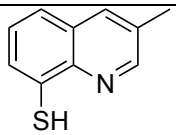
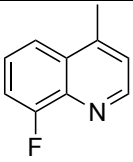
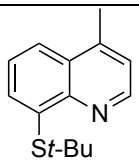
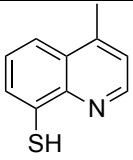
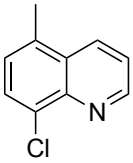
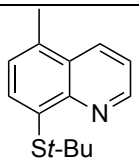
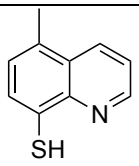
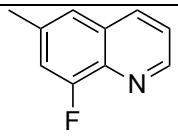
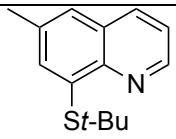
SUPPORTING INFORMATION

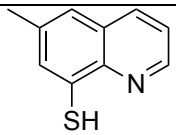
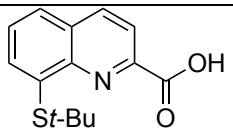
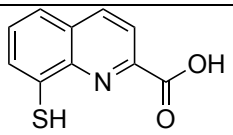
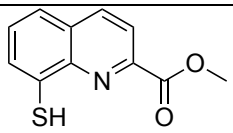
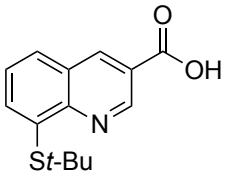
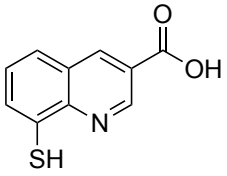
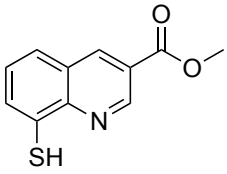
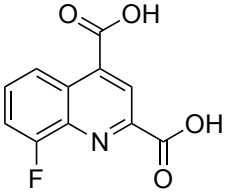
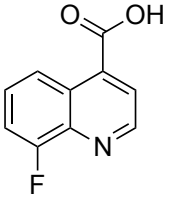
Contents

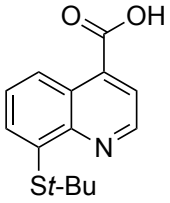
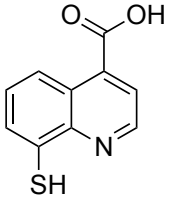
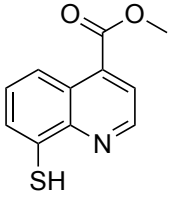
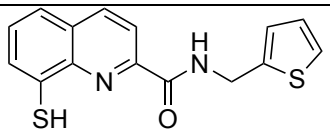
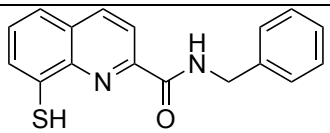
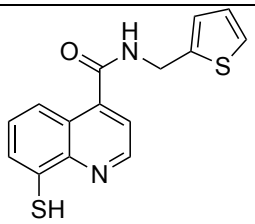
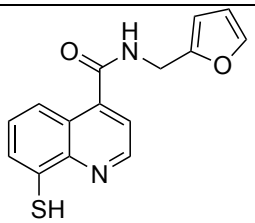
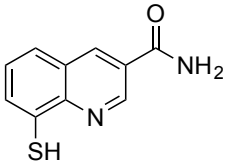
Compound Identification and Molecular Formula Strings

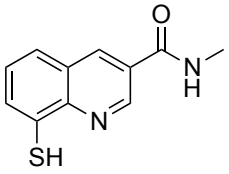
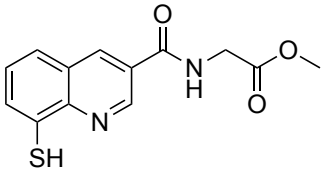
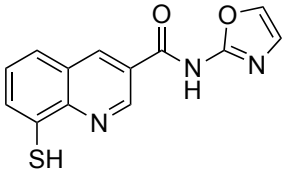
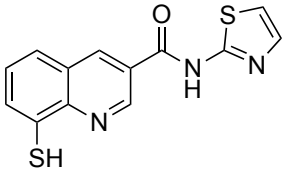
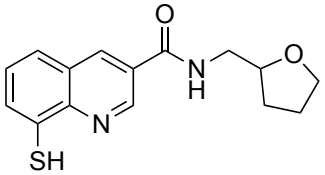
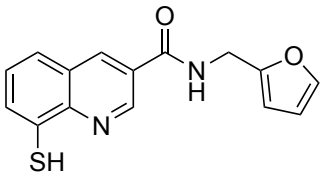
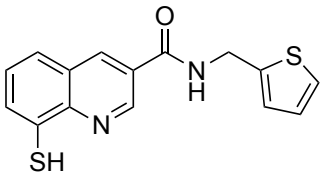
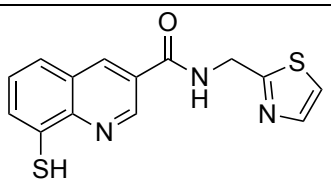
Cmpd Name	Structure	Catalog Name	SMILES
8TQ		**0001**	SC1=C(N=CC=C2)C2=CC=C1
2		**1000**	SC1=C(C=CC=C2)C2=CC=C1
3		**1005**	CC1=C(N=CC=C2)C2=CC=C1
4		**1003**	OC1=C(N=CC=C2)C2=CC=C1
5		**1004**	NC1=C(N=CC=C2)C2=CC=C1
6		**1002**	CSC1=C(N=CC=C2)C2=CC=C1
7a		**----**	ClC1=C(C=CC=N2)C2=CC=C1
7b		**----**	CC(C)(C)SC1=C(C=CC=N2)C2=CC=C1
7c		**1001**	SC1=C(C=CC=N2)C2=CC=C1

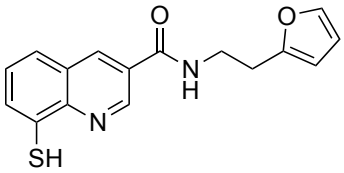
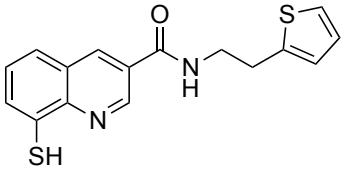
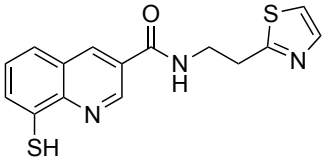
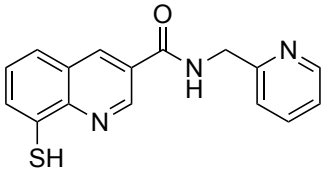
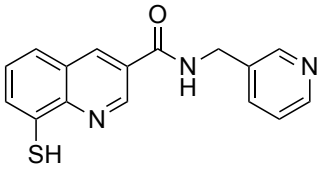
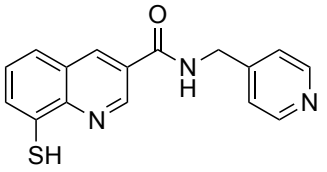
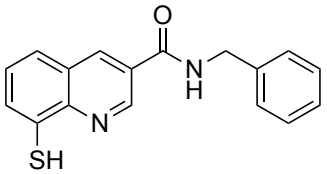
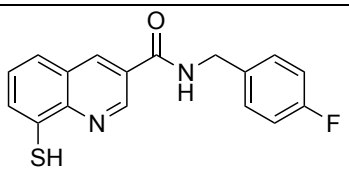
8a		**----**	CC(OC/1=O)(C)OC(C1=C/NC2=CN=CC=C2)=O
8b		**----**	OC1=CC=NC2=C1N=CC=C2
8c		**----**	ClC1=CC=NC2=C1N=CC=C2
8d		**----**	COC(C=C1)=CC=C1CSC2=CC=NC3=C2N=CC=C3
8e		**1011**	SC1=CC=NC2=C1N=CC=C2
9a		**----**	FC1=C(N=C(C)C=C2)C2=CC=C1
9b		**----**	CC1=NC2=C(SC(C)(C)C)C=CC=C2C=C1
9c		**1006**	SC1=C(N=C(C)C=C2)C2=CC=C1
10a		**----**	FC1=C(N=CC(C)=C2)C2=CC=C1
10b		**----**	CC1=CC2=CC=CC(SC(C)(C)C)=C2N=C1

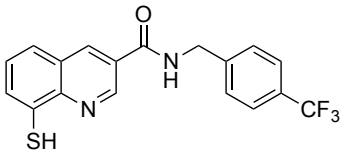
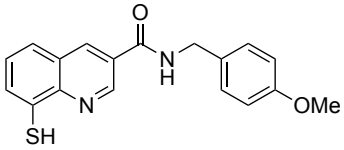
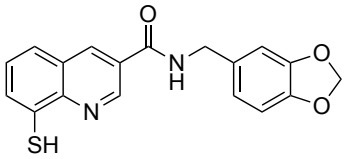
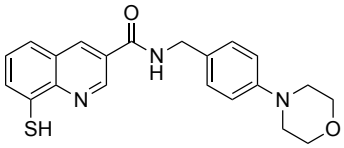
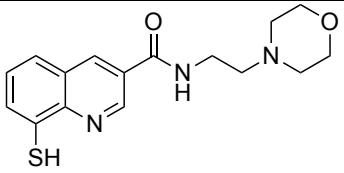
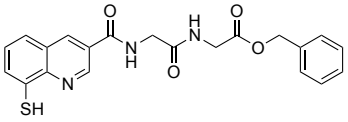
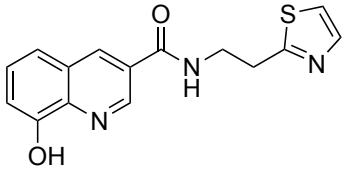
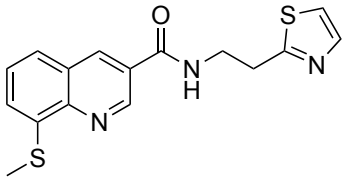
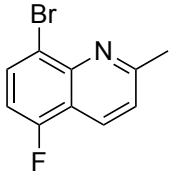
10c		**1007**	SC1=C(N=CC(C)=C2)C2=CC=C1
11a		**----**	FC1=C(N=CC=C2C)C2=CC=C1
11b		**----**	CC1=CC=NC2=C(SC(C)(C)C)C=CC=C21
11c		**1008**	SC1=C(N=CC=C2C)C2=CC=C1
12a		**----**	ClC1=C(N=CC=C2)C2=C(C)C=C1
12b		**----**	CC1=C2C(N=CC=C2)=C(SC(C)(C)C)C=C1
12c		**1009**	SC1=C(N=CC=C2)C2=C(C)C=C1
13a		**----**	FC1=C(N=CC=C2)C2=CC(C)=C1
13b		**----**	CC1=CC(SC(C)(C)C)=C(N=CC=C2)C2=C1

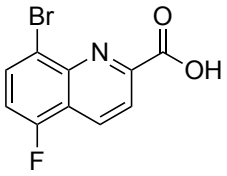
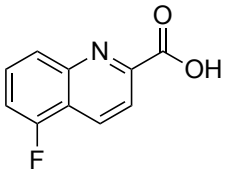
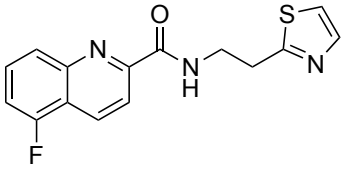
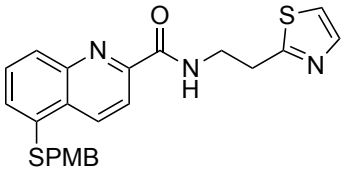
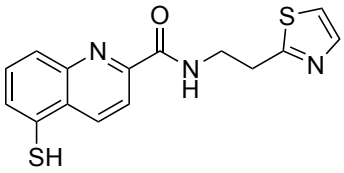
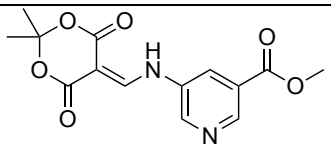
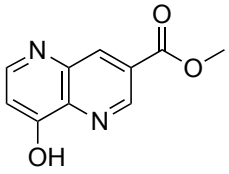
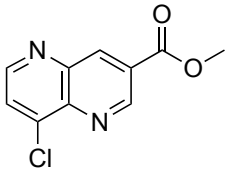
13c		**1010**	SC1=C(N=CC=C2)C2=CC(C)=C1
14a		**----**	OC(C1=NC2=C(SC(C)(C)C)C=CC=C2C=C1)=O
14b		**2001**	SC1=C(N=C(C(O)=O)C=C2)C2=CC=C1
15		**2002**	SC1=C(N=C(C(OC)=O)C=C2)C2=CC=C1
16a		**----**	O=C(O)C1=CC2=CC=CC(SC(C)(C)C)=C2N=C1
16b		**3001**	SC1=C(N=CC(C(O)=O)=C2)C2=CC=C1
17		**3002**	SC1=C(N=CC(C(OC)=O)=C2)C2=CC=C1
18a		**----**	FC1=C(N=C(C(O)=O)C=C2C(O)=O)C2=CC=C1
18b		**----**	FC1=C(N=CC=C2C(O)=O)C2=CC=C1

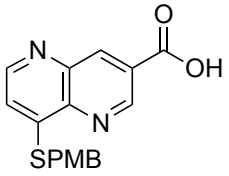
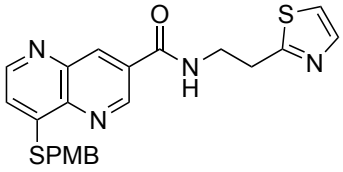
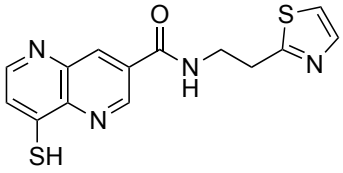
18c		**----**	O=C(O)C1=CC=NC2=C(SC(C)(C)C)C=CC=C21
18d		**4001**	SC1=C(N=CC=C2C(O)=O)C2=CC=C1
19		**4002**	SC1=C(N=CC=C2C(OC)=O)C2=CC=C1
20		**2003**	SC1=C(N=C(C(NCC2=CC=CS2)=O)C=C3)C3=CC=C1
21		**2004**	SC1=C(N=C(C(NCC2=CC=CC=C2)=O)C=C3)C3=CC=C1
22		**4004**	SC1=C(N=CC=C2C(NCC3=CC=CS3)=O)C2=CC=C1
23		**4006**	SC1=C(N=CC=C2C(NCC3=CC=CO3)=O)C2=CC=C1
24		**3003**	SC1=C(N=CC(C(N)=O)=C2)C2=CC=C1

25		**3004**	SC1=C(N=CC(C(NC)=O)=C2)C2=CC=C1
26		**3005**	SC1=C(N=CC(C(NCC(OC)=O)=O)=C2)C2=CC=C1
27		**3023**	SC1=C(N=CC(C(NC2=NC=CO2)=O)=C3)C3=CC=C1
28		**3021**	SC1=C(N=CC(C(NC2=NC=CS2)=O)=C3)C3=CC=C1
29		**3024**	SC1=C(N=CC(C(NCC2CCCO2)=O)=C3)C3=CC=C1
30		**3010**	SC1=C(N=CC(C(NCC2=CC=CO2)=O)=C3)C3=CC=C1
31		**3011**	SC1=C(N=CC(C(NCC2=CC=CS2)=O)=C3)C3=CC=C1
32		**3025**	SC1=C(N=CC(C(NCC2=NC=CS2)=O)=C3)C3=CC=C1

33		**3022**	SC1=C(N=CC(C(NCCC2=CC=CO2)=O)=C3)C3=CC=C1
34		**3018**	SC1=C(N=CC(C(NCCC2=CC=CS2)=O)=C3)C3=CC=C1
35		**3027**	SC1=C(N=CC(C(NCCC2=NC=CS2)=O)=C3)C3=CC=C1
36		**3007**	SC1=C(N=CC(C(NCC2=CC=CC=N2)=O)=C3)C3=CC=C1
37		**3008**	SC1=C(N=CC(C(NCC2=CC=CN=C2)=O)=C3)C3=CC=C1
38		**3009**	SC1=C(N=CC(C(NCC2=CC=NC=C2)=O)=C3)C3=CC=C1
39		**3006**	SC1=C(N=CC(C(NCC2=CC=CC=C2)=O)=C3)C3=CC=C1
40		**3015**	SC1=C(N=CC(C(NCC2=CC=C(F)C=C2)=O)=C3)C3=CC=C1

41		**3016**	SC1=C(N=CC(C(NCC2=CC=C(C(F)(F)F)C=C2)=O)=C3)C3=CC=C1
42		**3017**	SC1=C(N=CC(C(NCC2=CC=C(OC)C=C2)=O)=C3)C3=CC=C1
43		**3013**	SC1=C(N=CC(C(NCC2=CC=C(OCO3)C3=C2)=O)=C4)C4=CC=C1
44		**3019**	SC1=C(N=CC(C(NCC2=CC=C(N3CCOCC3)C=C2)=O)=C4)C4=CC=C1
45		**3012**	SC1=C(N=CC(C(NCCN2CCOCC2)=O)=C3)C3=CC=C1
46		**3014**	SC1=C(N=CC(C(NCC(NCC(OCC2=CC=CC=C2)=O)=O)=O)=C3)C3=CC=C1
47		**C001**	OC1=C(N=CC(C(NCCC2=NC=CS2)=O)=C3)C3=CC=C1
48		**C002**	O=C(NCCC1=NC=CS1)C2=CC3=CC=CC(SC)=C3N=C2
49a		**----**	FC1=C(C=CC(C)=N2)C2=C(Br)C=C1

49b		**----**	FC1=C(C=CC(C(O)=O)=N2)C2=C(Br)C=C1
49c		**----**	FC1=C(C=CC(C(O)=O)=N2)C2=CC=C1
49d		**----**	FC1=C(C=CC(C(NCCC2=NC=CS2)=O)=N3)C3=CC=C1
49e		**----**	O=C(NCCC1=NC=CS1)C2=NC3=CC=CC(SCC4=CC=C(OC)C=C4)=C3C=C2
49f		**C003**	SC1=C(C=CC(C(NCCC2=NC=CS2)=O)=N3)C3=CC=C1
50a		**----**	CC(OC/1=O)(C)OC(C1=C/NC2=CN=CC(C(OC)=O)=C2)=O
50b		**----**	OC1=CC=NC2=C1N=CC(C(OC)=O)=C2
50c		**----**	ClC1=CC=NC2=C1N=CC(C(OC)=O)=C2

50d		**----**	COC(C=C1)=CC=C1CSC2=CC=NC3=C2N=CC(C(O)=O)=C3
50e		**----**	COC(C=C1)=CC=C1CSC2=CC=NC3=C2N=CC(C(NCCC4=NC=CS4)=O)=C3
50f		**C004**	SC1=CC=NC2=C1N=CC(C(NCCC3=NC=CS3)=O)=C2

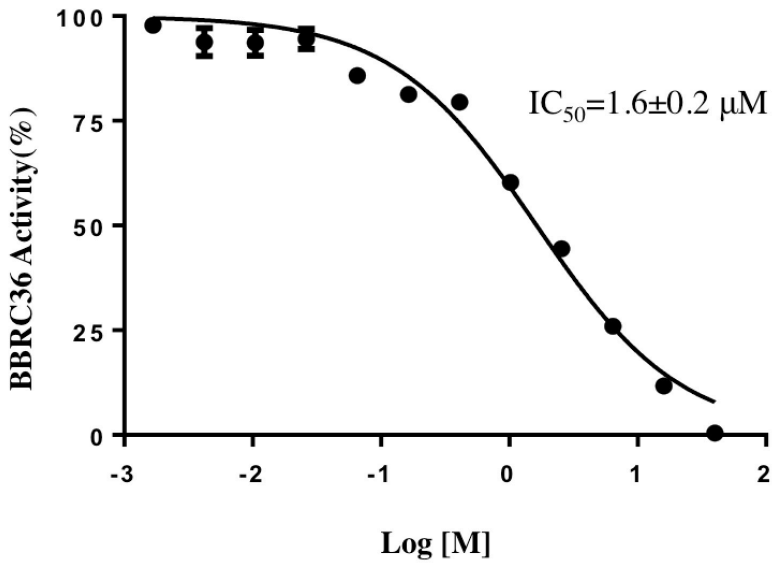


Figure S1. Inhibition of **8TQ** against the BBRC36 (BRISC) complex was measured. Error bars represent standard deviation (n = 4).